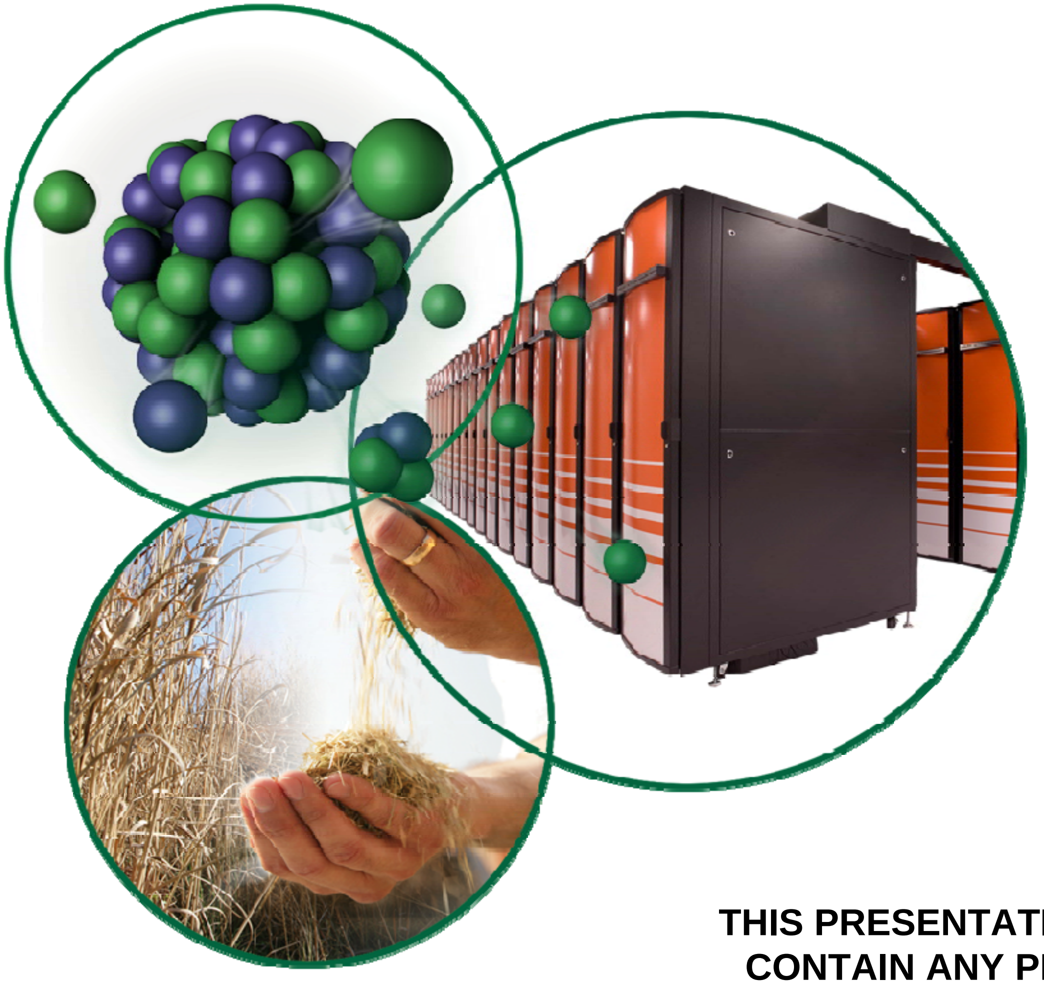
# Advanced Petroleum Based Fuel Effects in HCCI (Agreement 13415)



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**Research supported by DOE Fuel Technology Program, Kevin Stork and Dennis Smith are DOE management team**

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FEERC
Fuels, Engines, and Emissions Research Center



OAK RIDGE National Laboratory

# Advanced Petroleum Based Fuel Effects in HCCI

- **Goals and objectives**
- **2007 reviewer feedback**
- **Barriers addressed**
- **Approach**
- **Accomplishments**
- **Technology transfer**
- **Summary**
- **Activities for next year**

# Goals and objectives

- Define tradeoffs and performance of fuels in advanced combustion regimes to support decisions related to future fuels and engines with emphasis on:
  - Fuel economy
  - Fuel chemistry and properties
  - Engine control and emissions control
  - Both gasoline and diesel engines are being studied
- Advanced petroleum based fuels (APBF) are primarily derived from petroleum crude, but may utilize non-traditional processing and may contain non-petroleum components
- This is a companion project to another covering non-petroleum based fuels (NPBF) which is reported separately

# 2007 reviewer comments

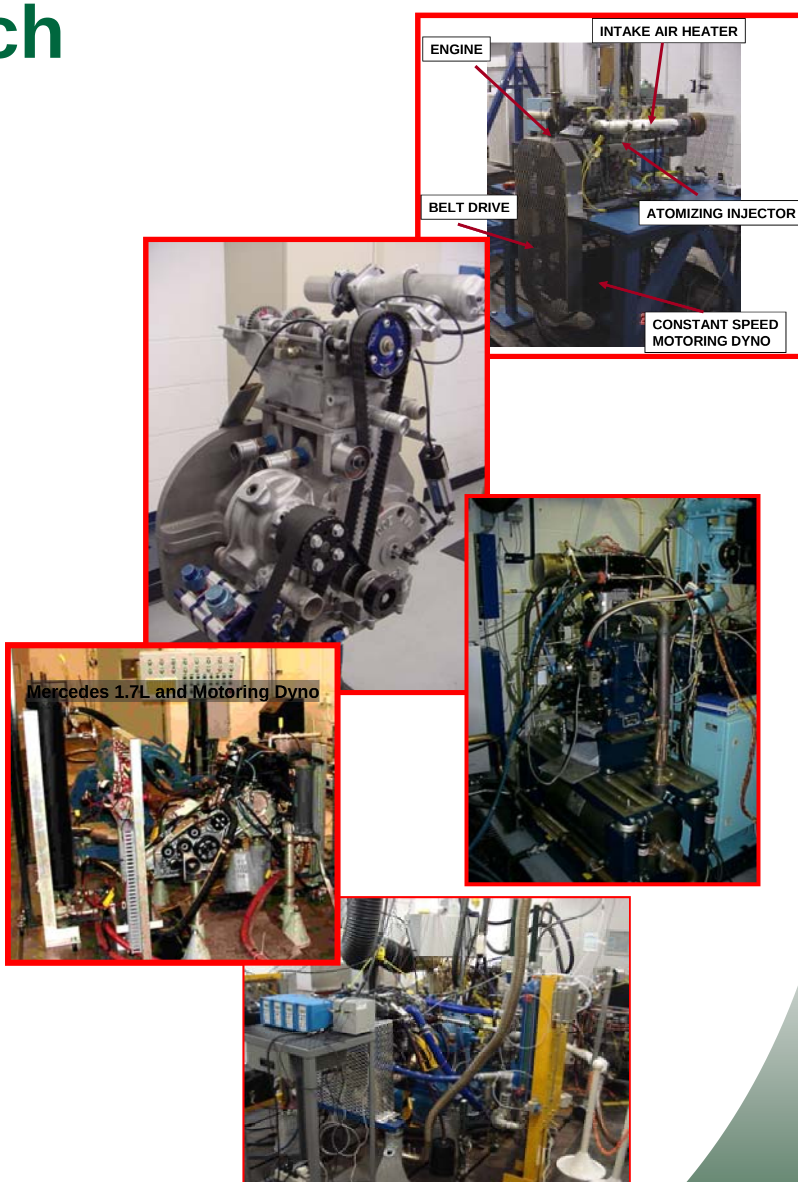
- **Expand studies to include surrogate fuels … more chemical or specific molecular effects … more bulk vs. species specific effects … pre-screening using kinetic modeling**
  - ***Added kinetic modeling and surrogates to research with refinery based fuels***
  - ***Added advanced statistics to allow performance analysis of complex, real fuels***
- **Get more students involved**
  - ***We are open to joint work, but have limited funding for university research. Please contact us with ideas or opportunities.***
- **Reviewer positive comments**
  - ***"Work is vital if LTC is to succeed, well aligned with DOE goals, tie between advanced combustion and fuel chemistry is essential, variety of fuels and engines being considered makes results universal, excellent database being created, good engagement and collaboration with energy companies and OEMs, focus on data mining and statistics is a good approach, comparing full boiling range fuels to surrogates is very valuable"***

# Barriers addressed

- The development of new engines and combustion regimes is being driven by need for greater fuel efficiency and reduced emissions
  – Research to date indicates that advanced combustion is more sensitive to fuel variations
- Fuels research is needed to support decisions about future fuels, new fuel sources, and development of advanced engines
- New engines will need to provide robust performance across a wider range of fuels and conditions
  – Greater diversity of fuel sources
  – ‘World engines’
- Engines will need ability to compensate for fuel changes

# Approach

- **Use a variety of research engines**
  - **Mercedes 1.7 and GM 1.9 for PCCI / HECC studies**
  - **Single cylinder engines for HCCI: to emphasize fuel effects and minimize fuel sample requirements**
- **Study wide variety of both refinery fuels and surrogate blends**
- **Use statistical analysis to mine data in order to develop a broader understanding of fuel behavior and to extract information relative to complex, market fuels**
- **Apply kinetic modeling as appropriate**



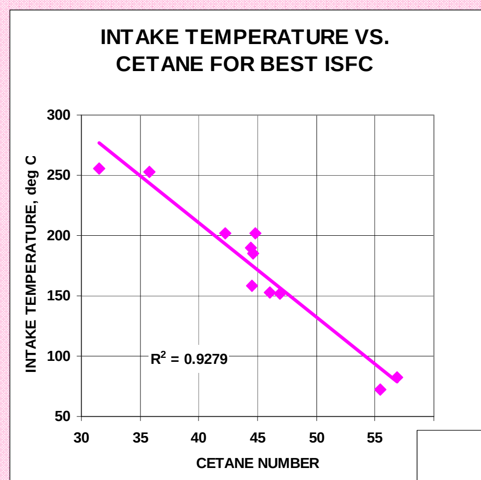
# Accomplishments / progress / results

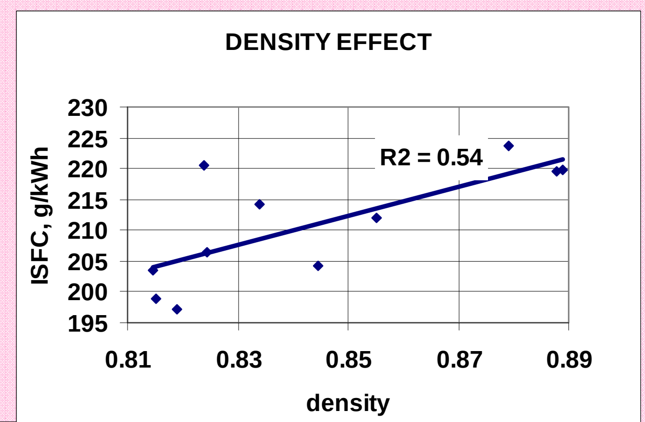
- Optimum engine efficiency is achieved by correctly matching a fuel to engine characteristics
  - Combustion phasing (MFB50) typically optimum at 5 to 10°ATDC
  - Must also avoid excessive rates of cylinder pressure rise and NOx and high levels of CO and HC due to combustion quenching
- Variable compression ratio is an effective control strategy for HCCI engines and is capable of rapid control changes
- Advanced statistical analysis (principal components analysis) is ideal for analyzing fuel and engine performance data to deal with the number of correlated variables typically found in real fuels
- Octane and cetane numbers remain major variables for fuel definition for HCCI, but fuel chemistry also plays a significant role in combustion characteristics
- CRADA with Reaction Design for Model Fuels Consortium provides access to kinetic modeling tools and another dimension of application for our fuels research data

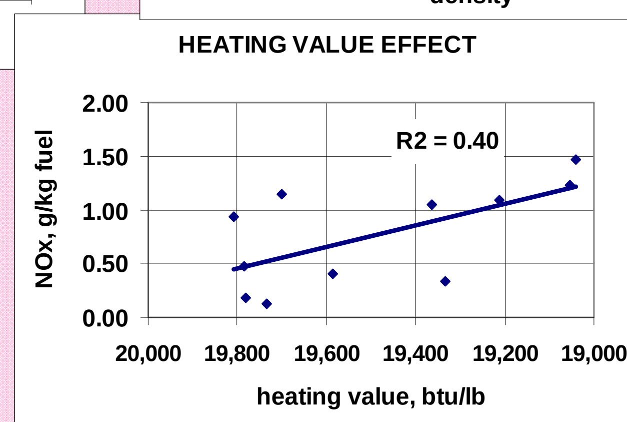
# Fuel effects and diesel HCCI

- **Engine management will need to compensate for fuel cetane number**
- **ISFC, ITE, and NOX all deteriorate with 'heavy' fuels**
  - Higher density
  - Higher T50
  - Higher aromatics
  - Lower LHV
- **Joint study with Cummins and BP**

| | CETANE | SPECIFIC GRAVITY | % MONO AROMATIC | % POLY AROMATIC | T50 | LHV |
|---|---|---|---|---|---|---|
| CETANE | 1.00 | | | | | |
| SPECIFIC GRAVITY | -0.41 | 1.00 | | | | |
| % MONO AROMATIC | -0.67 | 0.00 | 1.00 | | | |
| % POLY AROMATIC | -0.31 | 0.97 | -0.17 | 1.00 | | |
| T50 | 0.14 | 0.74 | -0.48 | 0.78 | 1.00 | |
| LHV | 0.59 | -0.96 | -0.25 | -0.90 | -0.56 | 1.00 |

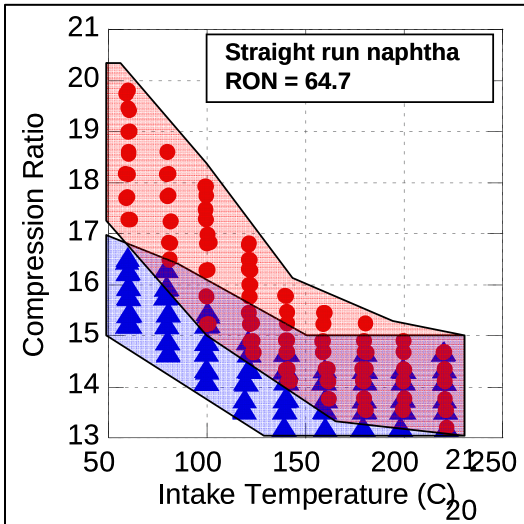


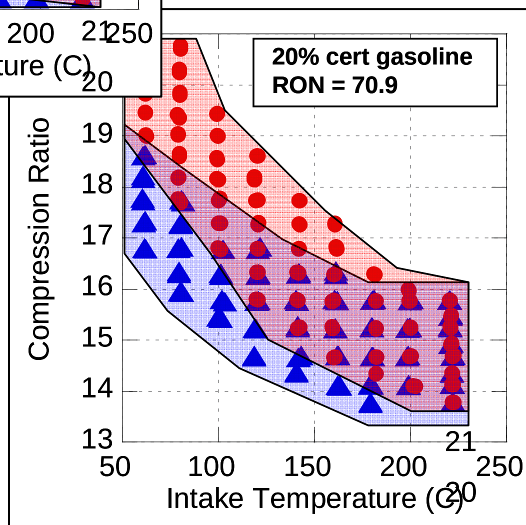



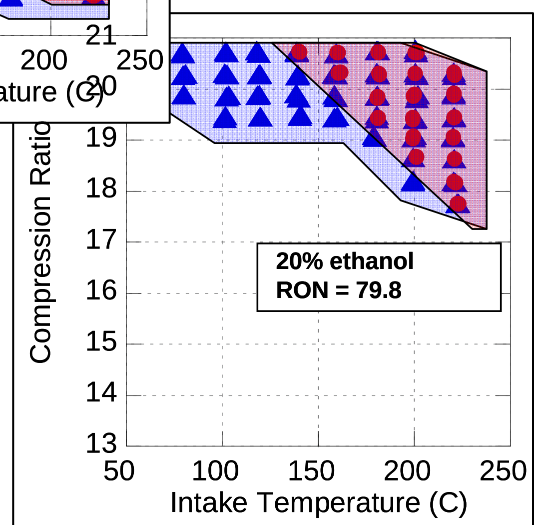



# Gasoline HCCI –
# VCR is a good control for HCCI

- **Temperature and CR are interchangeable for control**
- **VCR provides faster response than temperature**
- **Higher RON requires higher temperature and/or CR**
- **Un-throttled operation requires higher temperature and/or CR**



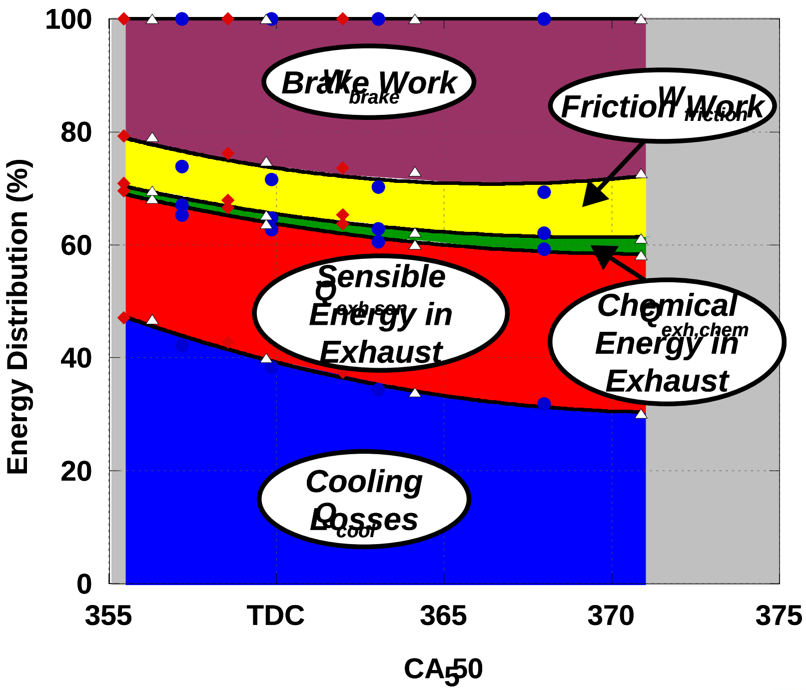



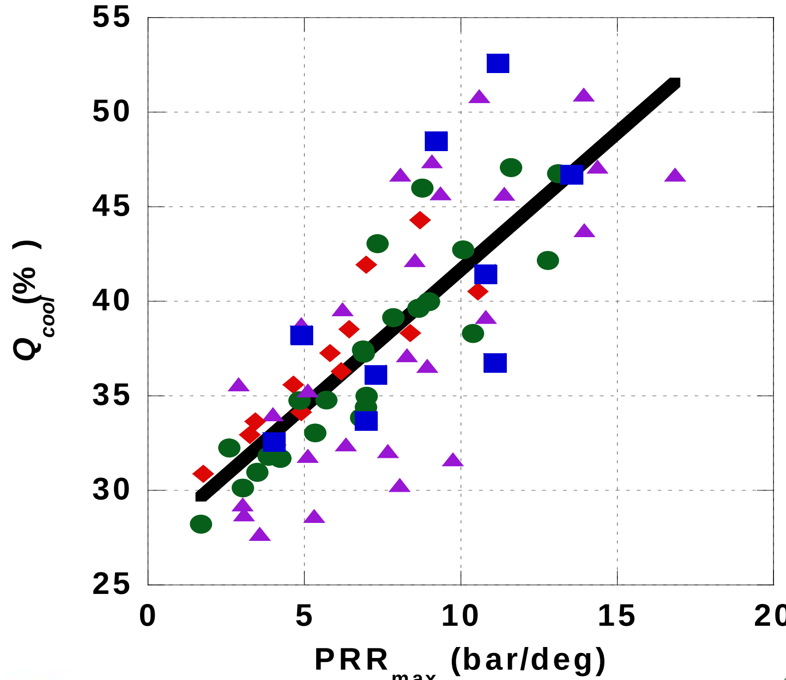




**Red = un-throttled (lambda 2.1 to 2.6)**
**Blue = constant lambda (2.1)**

# Effect of CR on efficiency is not ‘more is better’

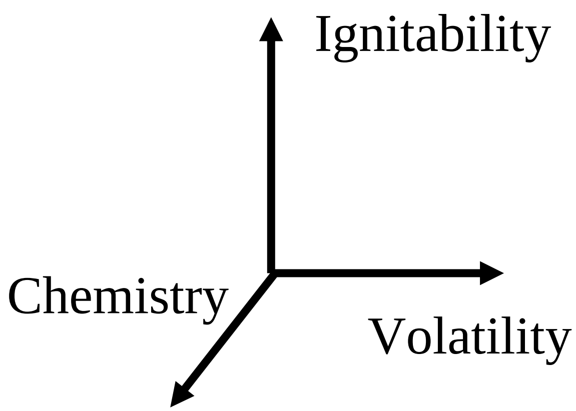
- **Efficiency increases with compression ratio, until rate of cylinder pressure rise increases heat loss from combustion chamber**
- **Cooling losses (from simple heat balance) increase with higher rate of cylinder pressure rise, which can occur from higher CR, more advanced timing, and/or higher intake temperature**

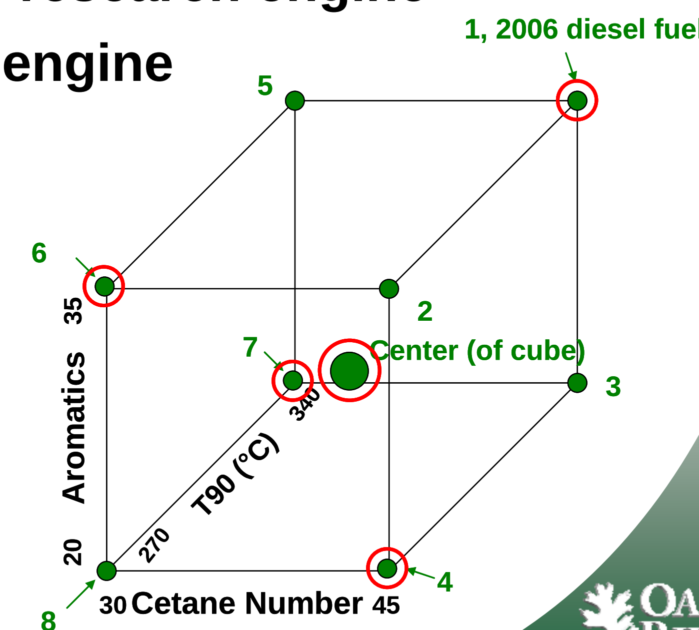


# FACE fuels - Fuels for advanced combustion engines

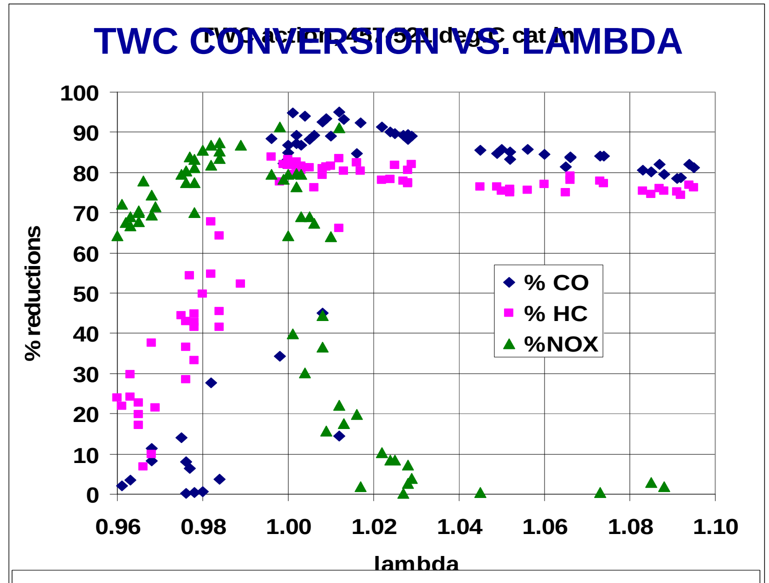
- DOE funded, CRC administrated, multiple national labs
- Specify and supply standard sets of diesel and gasoline fuels for advanced combustion research
  - Diesels designed, manufactured, in analysis
  - Gasolines designed, out for bid
- ORNL has diesel fuels in house
  - Running in HCCI on single cylinder research engine
  - Running in HECC on Mercedes 1.7 engine

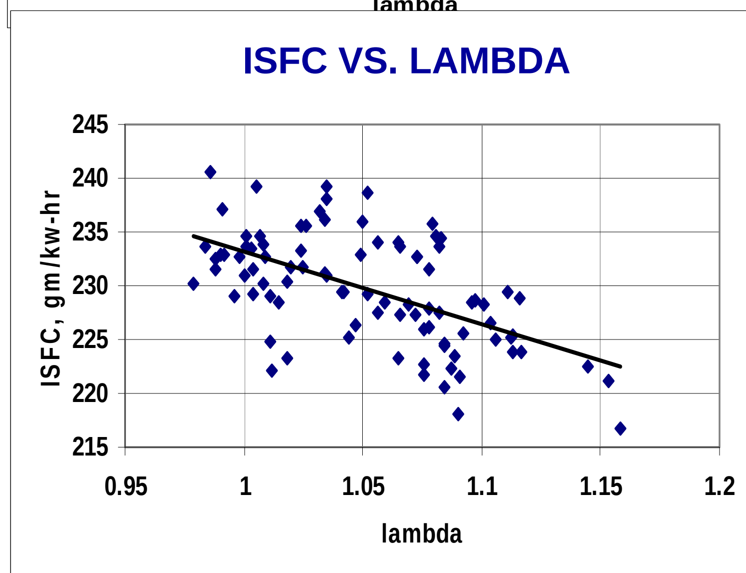


# Stoichiometric HCCI, ignition improvers, and TWC

- **Ignition improver (TBP, EHN) does improve gasoline HCCI ignition**
  - **High doses required – may not be commercially feasible**
  - **EHN also increases NOx emissions**
- **High EGR HCCI engines can be run at stoichiometric condition**
  - **Opens the door for use of TWC for high load NOx control and light load CO and HC control**
  - **Very challenging application for aged catalysts**
    - **Low exhaust temperatures**
    - **High CO and HC**
  - **Control issues with stoichiometric operation**
  - **Loss of fuel economy with stoichiometric operation**
- **Research results will be presented at Sandia MOU meeting next month**



# Advanced statistics for understanding fuels related data

- We are using principal components analysis (PCA)
  - Past use at ORNL for analysis of fuels and emissions data
  - Independent variables are resolved into orthogonal eigenvectors
  - Allows inclusion of all variables, it is not necessary to choose between multiple correlated variables
  - Maintains correlations between independent variables as they exist in the original data
  - Well suited for the analysis of fuels and engines, which often have multiple correlated variables
- We build model into a simulator format so that experiments can be ‘rerun’ on a computer to focus on specific effects or operating conditions
  - Still can’t extrapolate beyond limits of the experimental data
- Bonus project – re-analysis of AVFL13 HCCI gasoline results

# Cooperative research program with Reaction Design for Model Fuels Consortium

- Gain access to comprehensive set of kinetic modeling tools
- Provides another dimension of usefulness for our fuels and engine data
  - OEM and energy company members
  - Some results will be jointly published
- ORNL contribution - studies of diesel and gasoline range surrogate fuels
  - Mining of past data
  - Parametric modeling studies
  - Gasoline, diesel, and bio-fuel surrogate blend experiments
    - Gasoline experiments complete

# Technology transfer

- Funds-in project with Cummins and BP
  - HECC and HCCI fuel effects and engine optimization
- Funds-in project with major energy company
- CRADA with Reaction Design for Model Fuels Consortium
- Presentations, technical papers
- APBF/NPBF, Invited speaker at 4 fuels and combustion related workshops and symposia in 2007 (SAE HCCI Symposium, AOCS World Biodiesel Congress, Univ. of Wisconsin Future Fuels Symposium, and Oil Sands Research Roadmap Workshop)
- Reanalysis of AVFL13 data using PCA

# 2007 APBF/NPBF publications and presentations

- Bunting, Strategies for Optimization of Engines, Fuels, and Aftertreatment. ERC Research Symposium, University of Wisconsin, June 2007.
- Szybist, McFarlane, and Bunting, Comparison of Simulated and Experimental Combustion of Biodiesel Blends in a Single Cylinder Diesel HCCI Engine, SAE technical paper 2007-01-4010.
- Szybist and Bunting., The Use of Fuel Chemistry and Property Variations to Evaluate the Robustness of Variable Compression as a Control Method for Gasoline HCCI, SAE technical paper 2007-01-0224.
- Szybist and Bunting, The Effects of Fuel Composition and CR on Thermal Efficiency in an HCCI Engine, SAE paper 2007-01-4076.
- Bunting, Eaton, Szybist, Crawford, Yu, and Wolf, The Performance of B20 Biodiesels from a Variety of Sources in HCCI Combustion. Presented at the AOCS International Congress on Biodiesel, November 2007.
- Bunting, Wildman, Szybist, Lewis, and Storey, Fuel Chemistry and Cetane Effects on Diesel Homogeneous Charge Compression Ignition Performance, Combustion, and Emissions. International Journal of Engine Research, vol 8, p 15-27, 2007.
- Szybist and Bunting, Compression Ratio, Lambda, and Fuel Composition Effects on Gasoline-Range HCCI. Combustion MOU Presentation, February 2007.
- Oil sands research roadmap workshop, deer talk, presentation to diesel crosscut

# Summary

- **Optimum engine efficiency is achieved by correct matching of a fuel to engine characteristics**
  - **combustion phasing (MFB50) in the range of 5 to 10°ATDC**
  - **balance excessive rates of cylinder pressure rise and NOx against high levels of CO and HC due to combustion quenching**
- **Variable compression ratio is a effective combustion control strategy for HCCI engines and is capable of rapid control changes**
- **Advanced statistics in the form of PCA allows analysis of correlated fuel variables, which are often present in market fuels**
- **Octane and cetane numbers are major variables for fuel definition for HCCI, but fuel chemistry plays a larger role in than it does in conventional combustion**
- **The Reaction Design Model Fuels Consortium allows ORNL access to latest kinetic modeling tools and provides another avenue of application for ORNL fuels research data**

# Activities for next year

- Continue to study effects of fuel properties and chemistry on HCCI combustion for real and surrogate fuels
- Determine more definite rules for matching fuels and engines in order to achieve maximum fuel efficiency
- Develop understanding of how engines can be controlled to compensate for varying fuel properties in order to maximum economy while meeting other requirements
- Continue to mine past data as we learn new things

# Reviewer summary

- **Support goal of petroleum displacement**
  - ***Define performance characteristics of new fuels and new combustion regimes, with emphasis on fuel economy. Help support decision making about future directions.***
- **Approach**
  - ***Diverse engine platforms, wide range of fuels, surrogates and refinery fuels, statistical analysis, kinetic modeling***
- **Technical accomplishments and progress**
  - ***Match of engine and fuels to achieve optimum efficiency***
  - ***Wide range of fuels studied***
  - ***Multiple platforms***
- **Tech transfer / market transformation**
  - ***Funds-in projects, CRADA, publications***
- **Next year's plans**
  - ***Continue data mining, modeling, experimentation, efficiency analysis***
- **Noteworthy aspects / barriers**
  - ***Statistics applied to market fuels, surrogates and modeling for deeper understanding***